

ESTIMATION AND CONTROL OF MODELING AND DISCRETIZATION ERRORS IN STRUCTURAL AND SOLID MECHANICS

J. Tinsley Oden

Associate Vice President for Research
Director, Institute for Computational Engineering and Sciences
Cockrell Family Regents' Chair in Engineering
The University of Texas at Austin

**Workshop on Advanced Simulations
for Nuclear Fuel Cycles**

**Lawrence Livermore National Laboratory
Livermore, California
December 14-15, 2005**

Supported by DOE and ONR



ACES Building

OUTLINE

1. Review of the General Framework for Goal-Oriented Error Estimation and Control

- 1.1 Abstract Variational Formulation of the Base Model
- 1.2 The Error in the Quantity of Interest
- 1.3 Multi-Scale Modeling and the Surrogate Model
- 1.4 Error Estimation
- 1.5 The Goals Algorithms

2. Applications

- 2.1 Elastostatics of heterogeneous materials
- 2.2 Molecular Statics: the Quasi-Continuum Method

3. Concluding Remarks

1. INTRODUCTORY IDEAS

A physical event
is depicted by a
mathematical model:

$$A(u) = F, \quad \text{in } V'$$

A goal is to calculate a
quantity of interest:

$$Q(u) = ?$$

$$Q: V \longrightarrow \mathbb{R}$$

The problem is generally
unsolvable, so it is replaced
by a **surrogate** problem:

$$A_0(u_0) = F_0, \quad \text{in } V'$$

1) The (wrong) value of Q is:

$$Q(u_0) \neq Q(u)$$

2) Can we estimate the error?

$$\mathcal{E} = Q(u) - Q(u_0)$$

3) Can we adapt the surrogate
model and control the error?

1.1 VARIATIONAL FORMULATION OF THE BASE MODEL

Weak form of model problem:

Let $B(u; v) = \langle A(u), v \rangle$ and $F(v) = \langle F, v \rangle$. Then

Find $u \in V$ such that $B(u; v) = F(v), \quad \forall v \in V$

Optimal Control Problem for $Q: V \rightarrow \mathbb{R}$:

$$Q(u) = \inf_{v \in M} Q(v)$$

$$M = \{v : B(v; w) = F(w), \forall w \in V\}$$

Then

$$\begin{aligned} B(u; q) &= F(q), & \forall q \in V & \text{(Primal)} \\ B'(u; v, p) &= Q'(u; v), & \forall v \in V & \text{(Dual)} \end{aligned}$$

1.2 ERROR FUNCTIONS AND RESIDUALS

Recall:

$$Q'(u; v) = \lim_{\theta \rightarrow 0} \theta^{-1} [Q(u + \theta v) - Q(u)]$$

$$B'(u; v, w) = \lim_{\theta \rightarrow 0} \theta^{-1} [B(u + \theta v; w) - B(u; w)]$$

Let (u_0, p_0) be an arbitrary pair on $V \times V$.

Denote the modeling errors:

$$e_0 = u - u_0, \quad \varepsilon_0 = p - p_0$$

and the residuals:

$$\mathcal{R}(u_0; q) = F(q) - B(u_0; q), \quad q \in V$$

$$\overline{\mathcal{R}}(u_0, p_0; v) = Q'(u_0; v) - B'(u_0; v, p_0), \quad v \in V$$

1.2 ERROR IN THE QUANTITY OF INTEREST

THEOREM¹: Given any approximation (u_0, p_0) of (u, p) ,

$$Q(u) - Q(u_0) = \mathcal{R}(u_0; p_0) + \mathcal{R}(u_0; \varepsilon_0) + \Delta(e_0, \varepsilon_0)$$

where

$$\begin{aligned} \Delta(e_0, \varepsilon_0) &= \frac{1}{2} \int_0^1 \left[Q'''(u_0 + se_0; e_0, e_0, e_0) \right. \\ &\quad - B'''(u_0 + se_0; e_0, e_0, e_0, p_0 + s\varepsilon_0) \\ &\quad \left. - 3B''(u_0 + se_0; e_0, e_0, \varepsilon_0) \right] (s-1)s \, ds \\ &+ \int_0^1 \left[B''(u_0 + se_0; e_0, e_0, p_0 + s\varepsilon_0) \right. \\ &\quad \left. - Q''(u_0 + se_0; e_0, e_0) \right] ds \end{aligned}$$

¹Oden & Prudhomme, *J. Comp. Phys.* (2002).

*For FEM's, see Oden & Prudhomme (1999), Rannacher & Becker (2001).

1.3 THE SURROGATE MODEL

Coarse or Surrogate Primal and Dual problems:

$$\begin{aligned} B_0(u_0; q) &= F_0(q), & \forall q \in V_0 \\ B'_0(u_0; v, p_0) &= Q'_0(u_0; v), & \forall v \in V_0 \end{aligned}$$

where $V_0 \subseteq V$ (analysis of modeling error).

Discrete Primal and Dual problems:

$$\begin{aligned} B_0(u_0^h; q^h) &= F_0(q^h), & \forall q^h \in V_0^h \\ B'_0(u_0^h; v^h, p_0^h) &= Q'_0(u_0^h; v^h), & \forall v^h \in V_0^h \end{aligned}$$

where $V_0^h \subset V_0$ (analysis of discretization error).

1.4 ERROR ESTIMATION

$$Q(u) - Q(u_0) = \mathcal{R}(u_0; p) \approx \mathcal{R}(u_0; \tilde{p})$$

Note that u_0 is rarely computed exactly. In general, only an approximation u_0^h to u_0 is available. In this case, we have:

$$Q(u) - Q(u_0^h) \approx \mathcal{R}(u_0^h; \tilde{p})$$

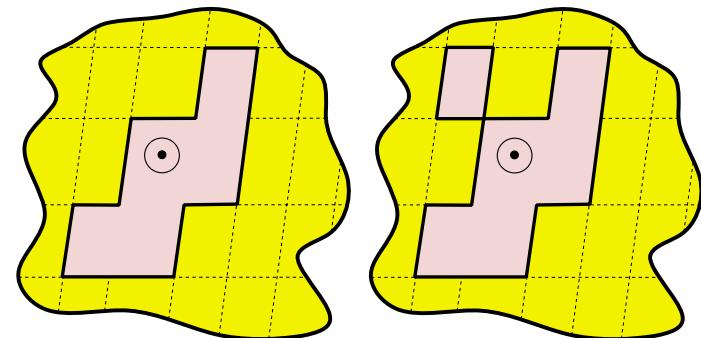
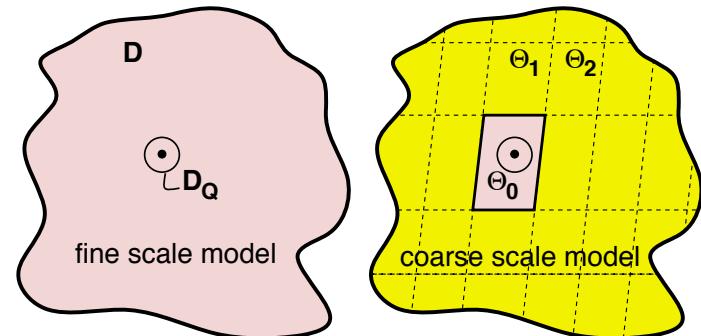
$$Q(u_0) - Q(u_0^h) \approx \mathcal{R}_0(u_0^h; \tilde{p}_0)$$

and

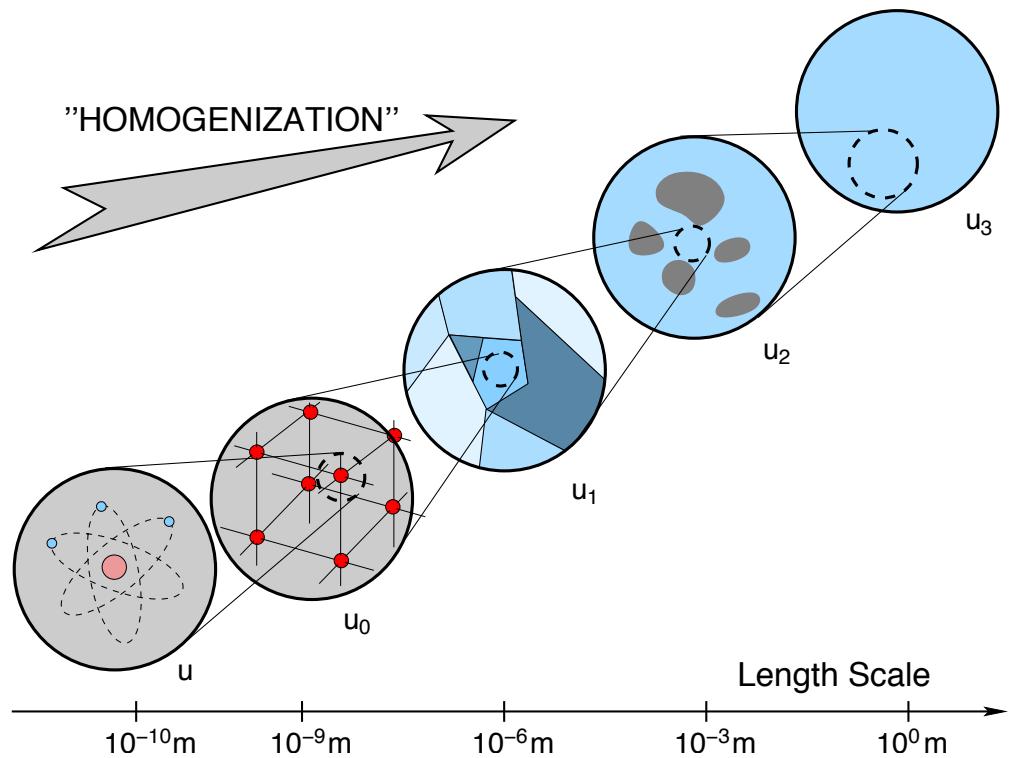
$$\underbrace{Q(u) - Q(u_0)}_{\text{modeling error}} = \underbrace{(Q(u) - Q(u_0^h))}_{\text{total error}} - \underbrace{(Q(u_0) - Q(u_0^h))}_{\text{discretization error}}$$

1.5 THE GOALS ALGORITHMS (2 SCALE SYSTEM)

- 1.** Let $D \subset \mathbb{R}^d$ and let $\{\Theta\}_{j=0}^k$ be a partition of D .
- 2.** Compute u_0 and $\mathcal{R}(u_0, p_0) \approx \mathcal{E}(u_0)$.
- 3.** Check $|\mathcal{E}(u_0)| \leq \delta_{\text{TOL}}$.
- 4.** Compute corrections (\tilde{u}, \tilde{p}) of (u_0, p_0) and continue until $|\mathcal{E}(u_0)| \leq \delta_{\text{TOL}}$.



1.5 MULTI-SCALE MODELING



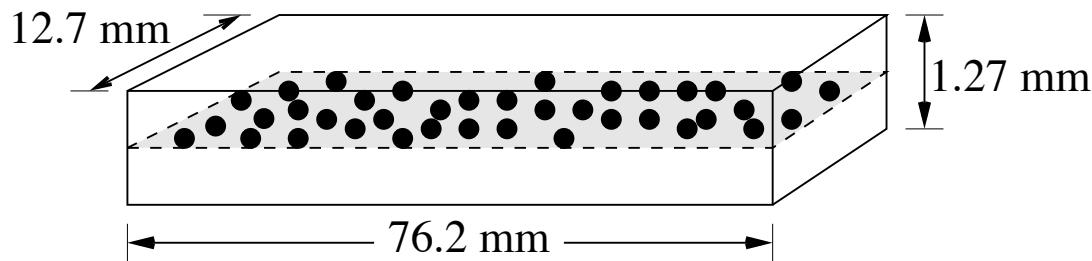
Major Open Problem:
Find homogenized model with $Q(u_0)$ close to $Q(u)$

$$Q(u) - Q(u_3) = \underbrace{Q(u) - Q(u_0)} + \underbrace{Q(u_0) - Q(u_1)} + \underbrace{Q(u_1) - Q(u_2)} + \underbrace{Q(u_2) - Q(u_3)}$$

2.1 APPLICATIONS - EPOXY/GLASS STRIP (EG)

Specimen description

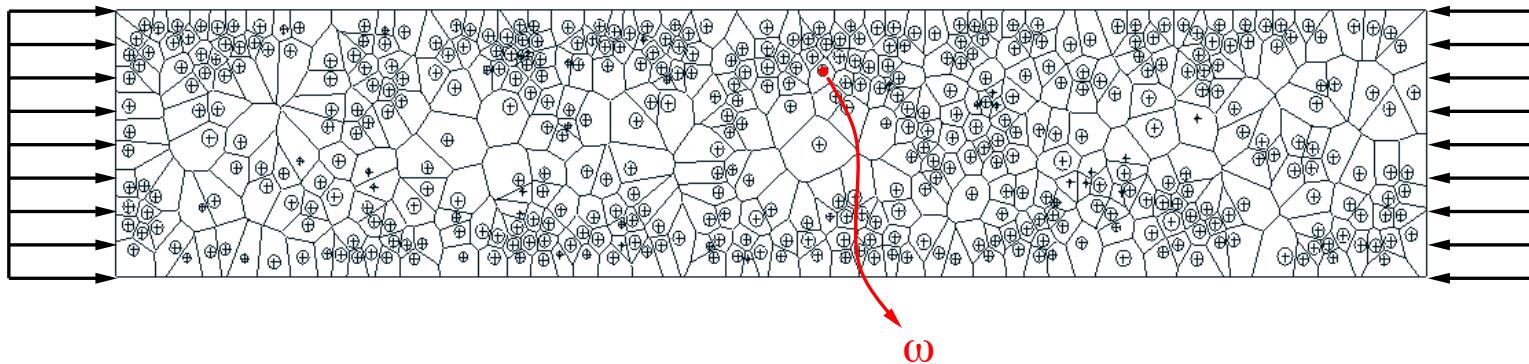
- ☞ Matrix material: Epoxy
- ☞ Inclusions: Single layer of Glass beads
- ☞ Average diameter of beads: $800 \mu\text{m}$
- ☞ CT resolution: $10 \mu\text{m}$
- ☞ Optical resolution: $1 \mu\text{m}$



* Vemaganti and Oden, CMAME (2000)

2.1 APPLICATIONS - EG EXAMPLE

Problem description



$$Q(v) = \int_{\omega} \sigma_{xx}(v) \, dx$$

Number of inclusions = 465

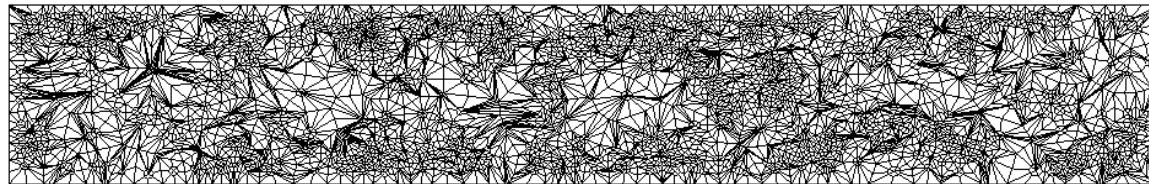
Epoxy: $E = 4.6 \text{ GPa}$, $\nu = 0.36$

Glass: $E = 69.0 \text{ GPa}$, $\nu = 0.22$

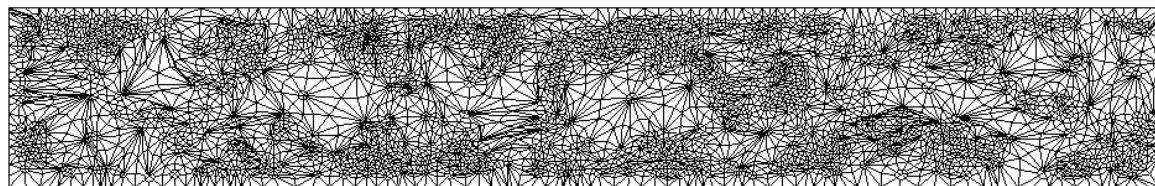
2.1 APPLICATIONS - EG EXAMPLE

Fine-scale Mesh

Initial Mesh:

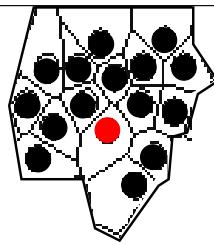


Mesh after Smoothing:

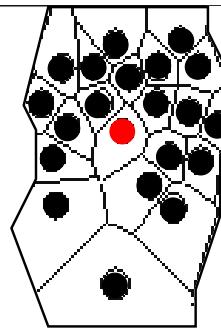


2.1 APPLICATIONS - EG EXAMPLE

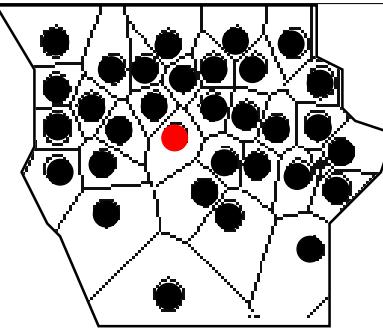
Relative Errors in Local Solution



17.0 %

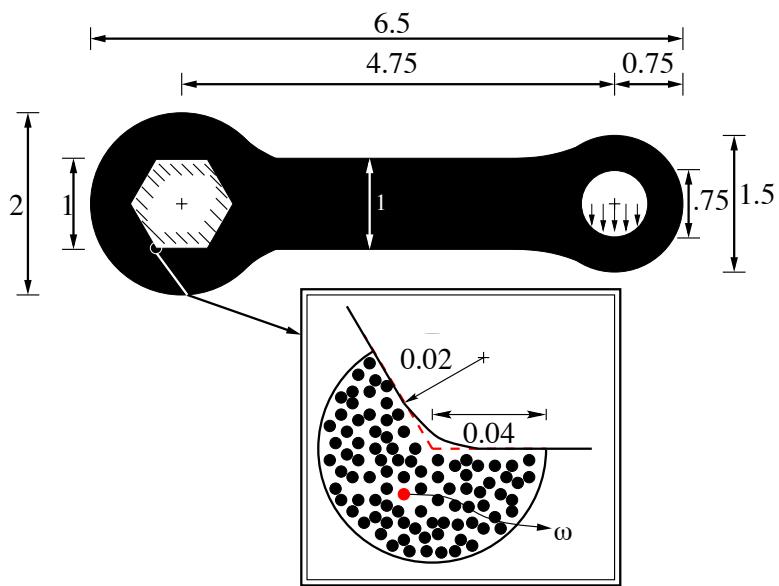


9.05 %



2.10 %

2.1 APPLICATIONS - COMPOSITE WRENCH

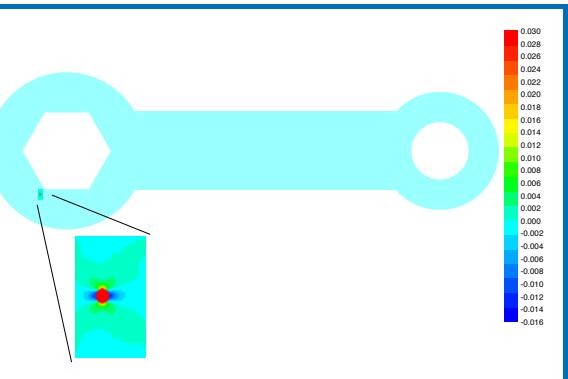
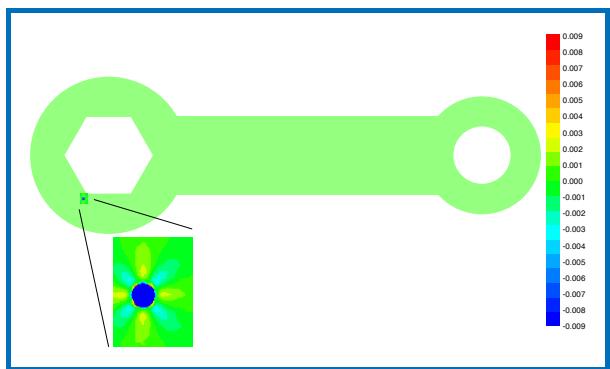


$$Q(v) = \frac{1}{|\omega|} \int_{\omega} \sigma_{xx}(v) dx$$

- 1. Microstructure is only known locally.**
- 2. Estimated number of inclusions in wrench = 128,000.**
- 3. Local volume fraction of inclusions = 0.4.**

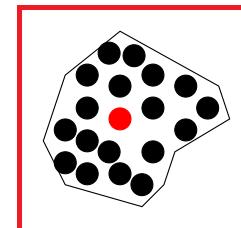
2.1 APPLICATIONS - COMPOSITE WRENCH

Influence Function

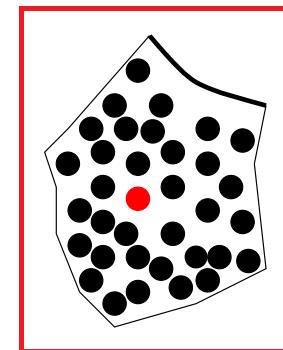


(T) $\varepsilon_{xx}(w^0)$, (B) $\varepsilon_{yy}(w^0)$

Adaptive Modeling

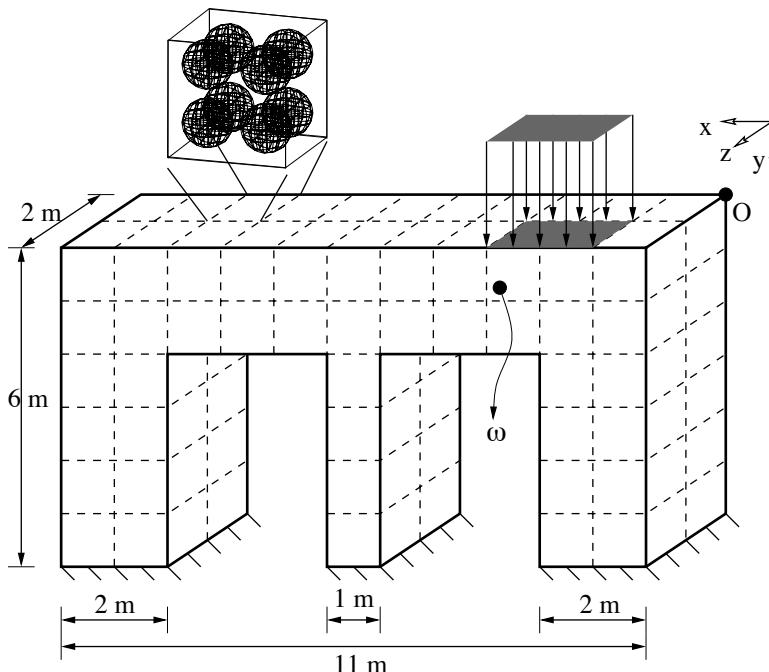


Estimated final
error = 12.2%



Estimated final
error = 4.2%

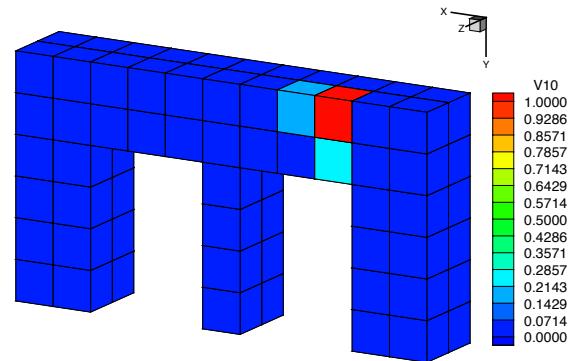
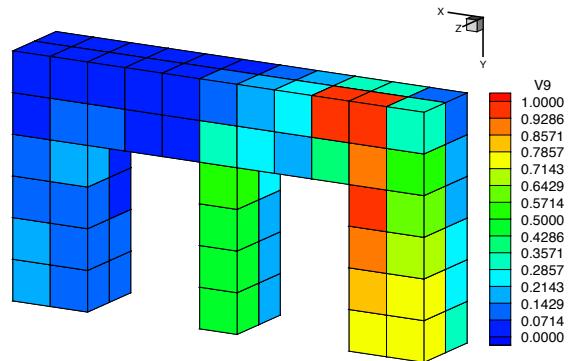
2.1 APPLICATIONS - 3-D EXAMPLE



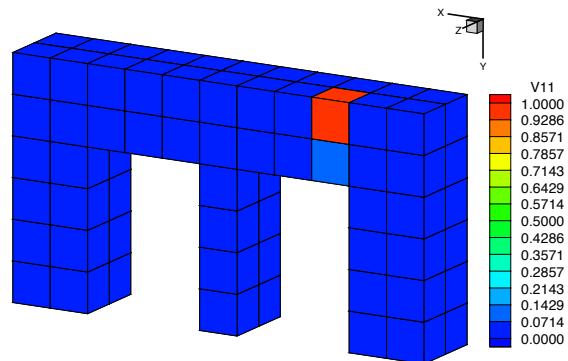
$$Q(v) = \frac{1}{\omega} \int_{\omega} \sigma_{22}(v) dx$$

Volume fraction of inclusions = 0.3; Stiffness ratio = 10

2.1 APPLICATIONS - 3-D EXAMPLE



ζ_k



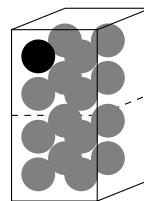
$\bar{\zeta}_k$

**Modeling Error
Distribution:
Normalized Modeling
Error Indicators**

β_k

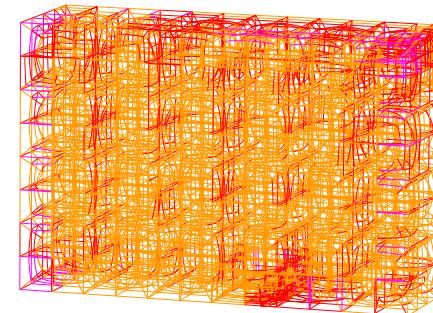
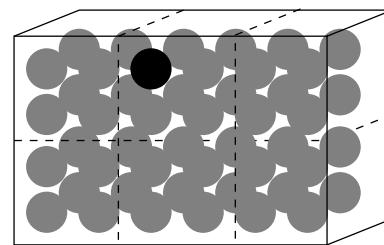
2.1 APPLICATIONS - 3-D EXAMPLE

Adaptive Modeling



P-Levels: 1 2 3 4 5 6 7 8

Estimated Error = 10%; 81,000 DOFs

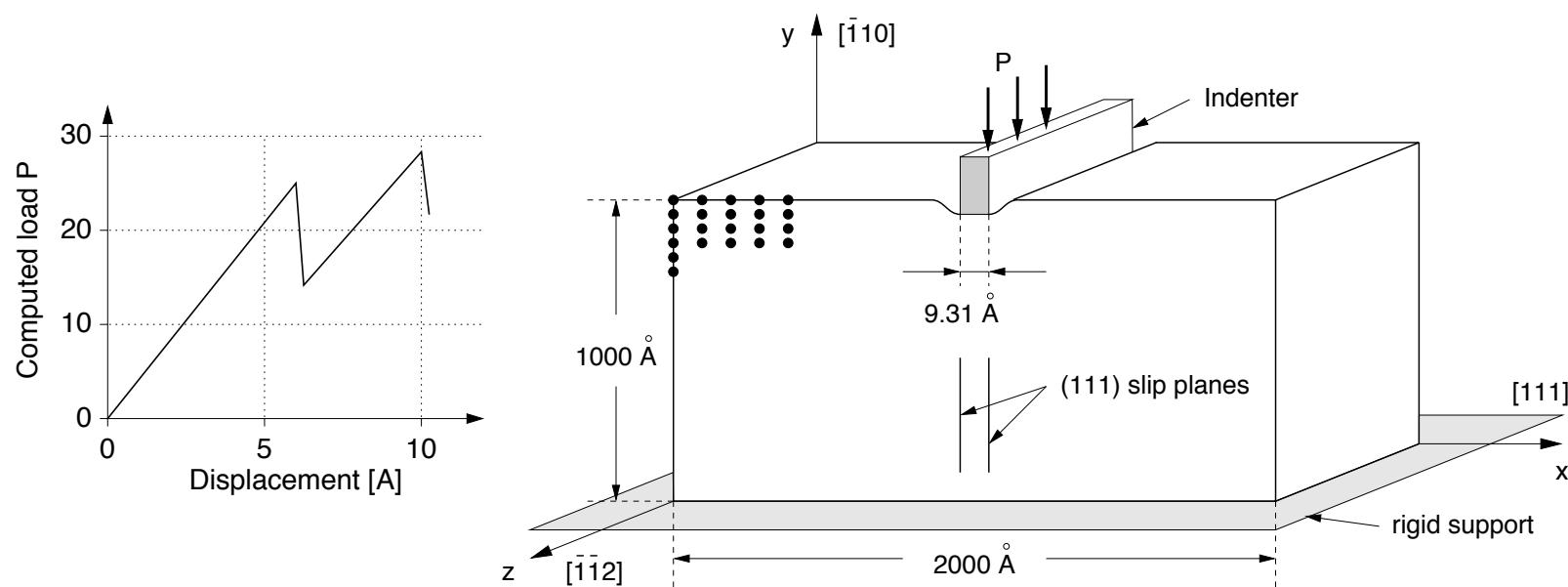


P-Levels: 1 2 3 4 5 6 7 8

Estimated Error = 4%; 130,000 DOFs

2.2 MOLECULAR STATIC EXAMPLE*

Nano-indentation of a thin aluminium film to study the initial stages of plastic deformation under the action of an indenter.



*Tadmor, Miller, Phillips, and Ortiz, J. Mat. Res. 14, (1999)

*Phillips, Rodney, Shenoy, Tadmor, and Ortiz, Model. Simul. Mat. Sci. Eng. 7 (1999)

2.2 THE BASE MODEL

Find $u \in \mathcal{V}$ and $p \in \mathcal{V}$ such that

$$\text{(Primal problem)} \quad \mathcal{B}(u; v) = \mathcal{F}(v), \quad \forall v \in \mathcal{V}$$

$$\text{(Dual problem)} \quad \mathcal{B}'(u; v, p) = Q'(u; v), \quad \forall v \in \mathcal{V}$$

where

$$\mathcal{B}(u; v) = \sum_{i=1}^N \left[\sum_{k=1}^N \frac{\partial E_k}{\partial u_i}(u) \right] \cdot v_i$$

$$\mathcal{F}(v) = \sum_{i=1}^N f_i \cdot v_i$$

and

$$\mathcal{B}'(u; v, p) = \sum_{j=1}^N \sum_{i=1}^N v_j \cdot \left[\sum_{k=1}^N \frac{\partial^2 E_k}{\partial u_j \partial u_i}(u) \right] \cdot p_i$$

2.2 THE SURROGATE MODEL BY QCM

The Quasi-Continuum Method (QCM)*

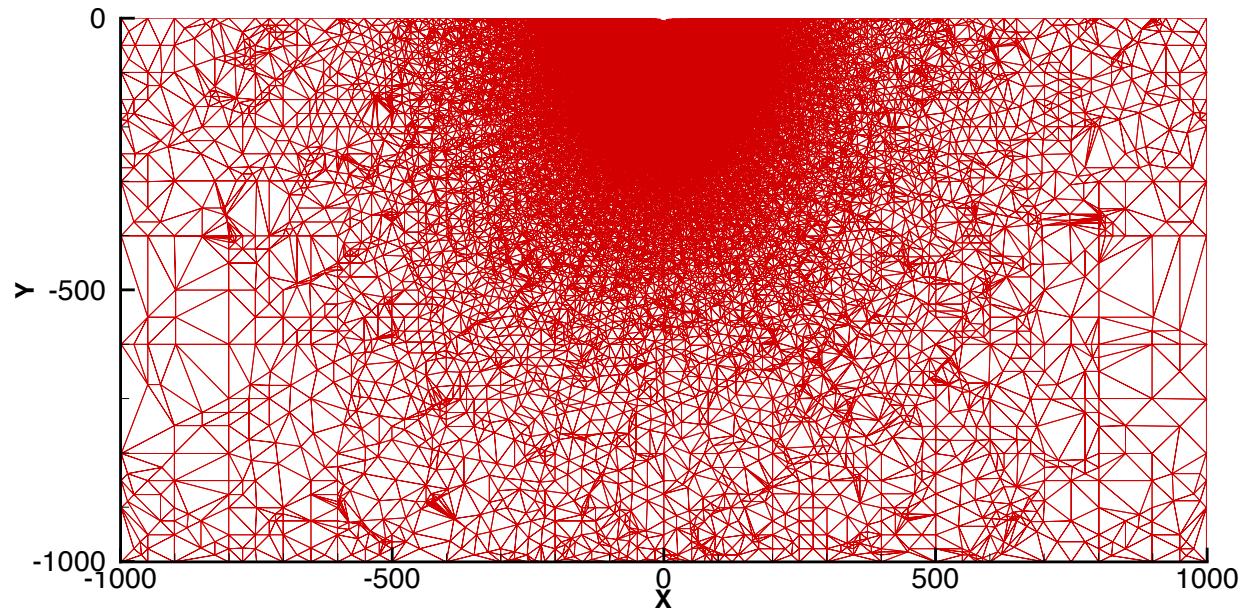
The goal of QCM is to find the atomic displacements that minimize the total potential energy such that:

1. The number of dofs is substantially reduced from $N \times d$.
2. The calculation of E_p is accurately approximated without the need to explicitly compute the site energies E_k of all the atoms.
3. The active dofs are adaptively selected to capture the critical deformations of the lattice.

The QCM belongs to the class of “concurrent methods”.

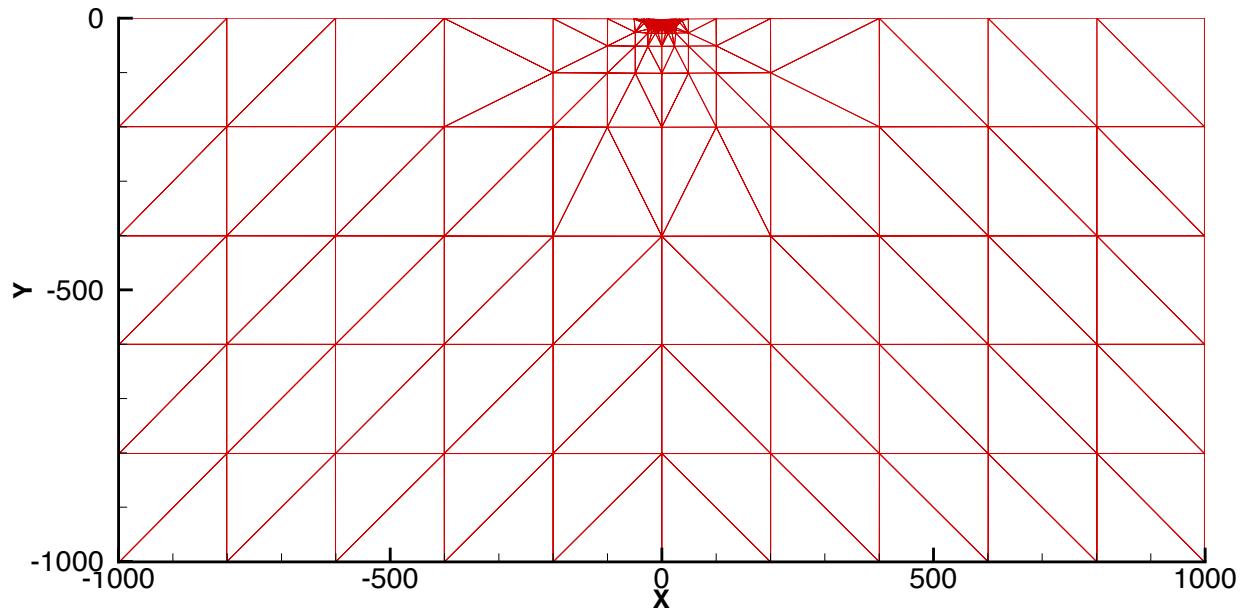
*Tadmor, diss. (1996), <http://www.qcmethod.com/>

2.2 BASE MODEL SOLUTION



**Finite element triangulation for the base model solution
at load step 26:
the mesh has 40554 active atoms.**

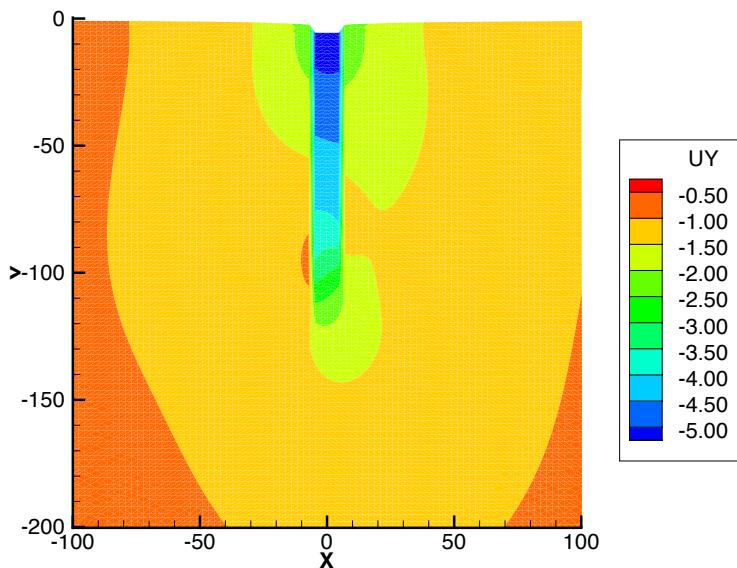
2.2 QUASICONTINUUM SOLUTION



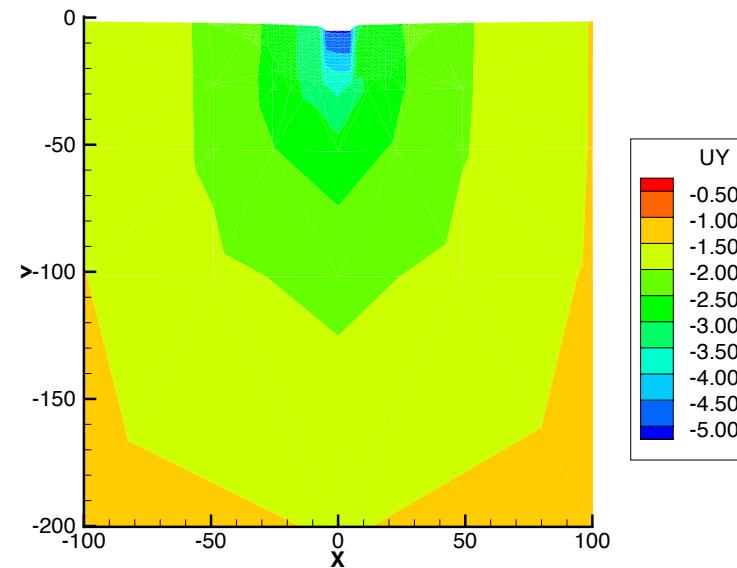
**Finite element triangulation for the QC solution
at load step 25:
the mesh has 492 active atoms.**

2.2 BASE AND QC SOLUTIONS

Displacement in y -direction
at dislocation nucleation



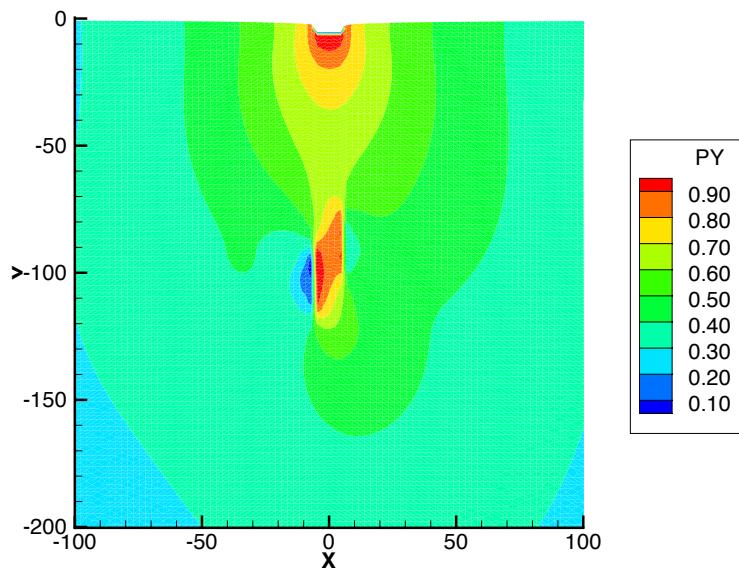
Base solution



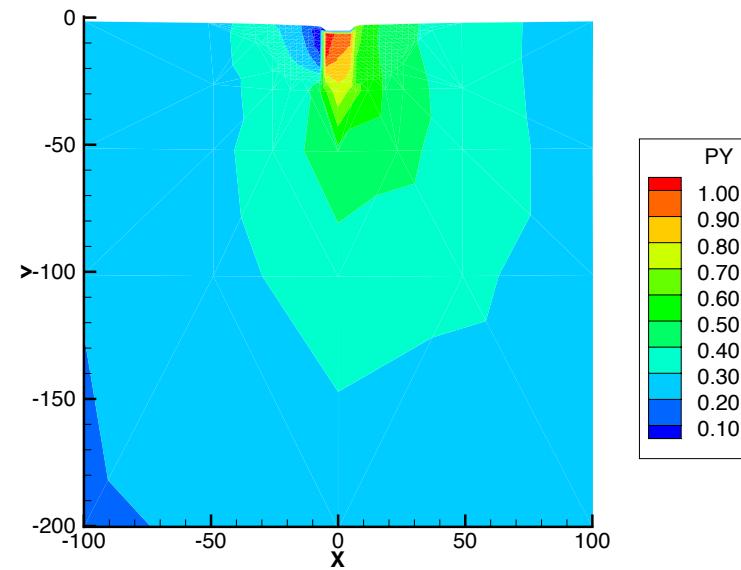
QC solution

2.2 BASE AND QC DUAL SOLUTIONS

Displacement in y -direction
at dislocation nucleation

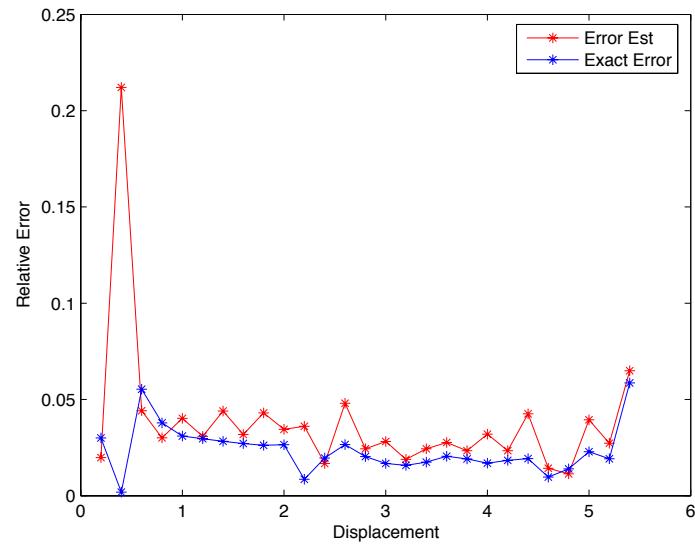
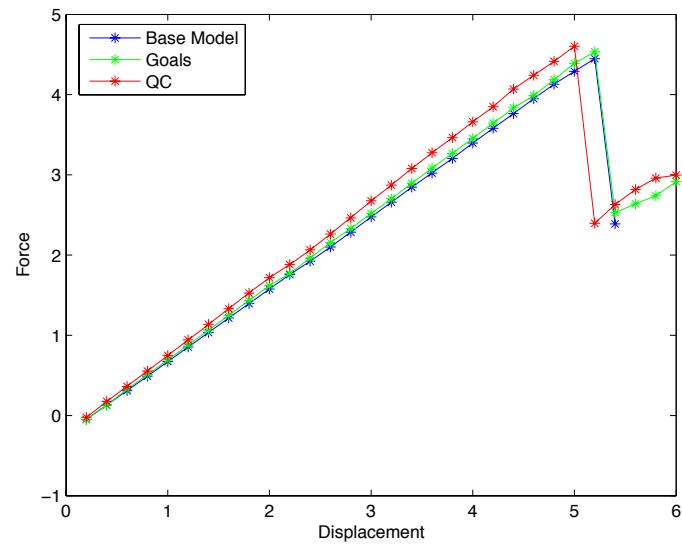


Base dual solution



QC dual solution

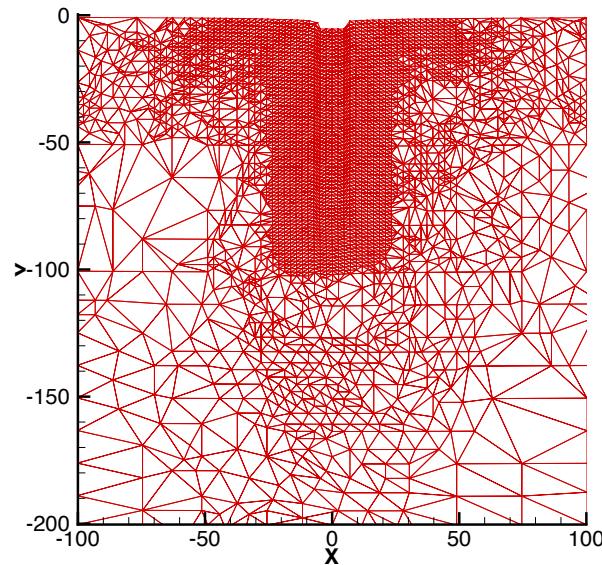
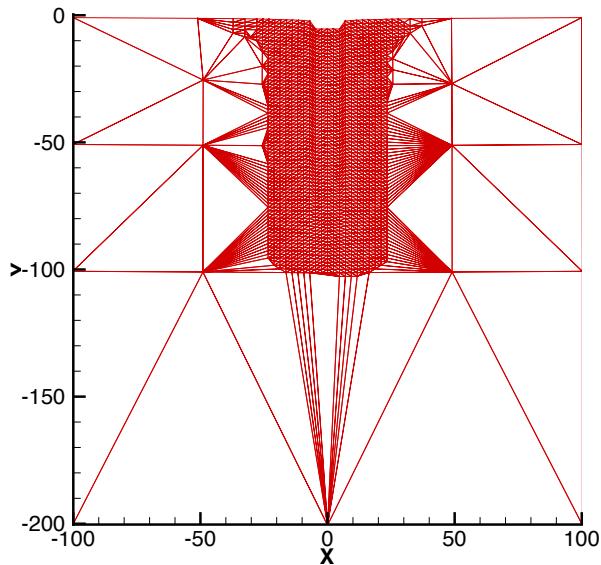
2.2 FORCE-DISPLACEMENT AND ERROR CURVES



(Left) Force-displacement curve comparing the evolution of the base model, QC, and Goals solutions.

(Right) Exact and estimated relative errors for the Goals solution.

2.2 QC AND GOALS MESH ADAPTATION



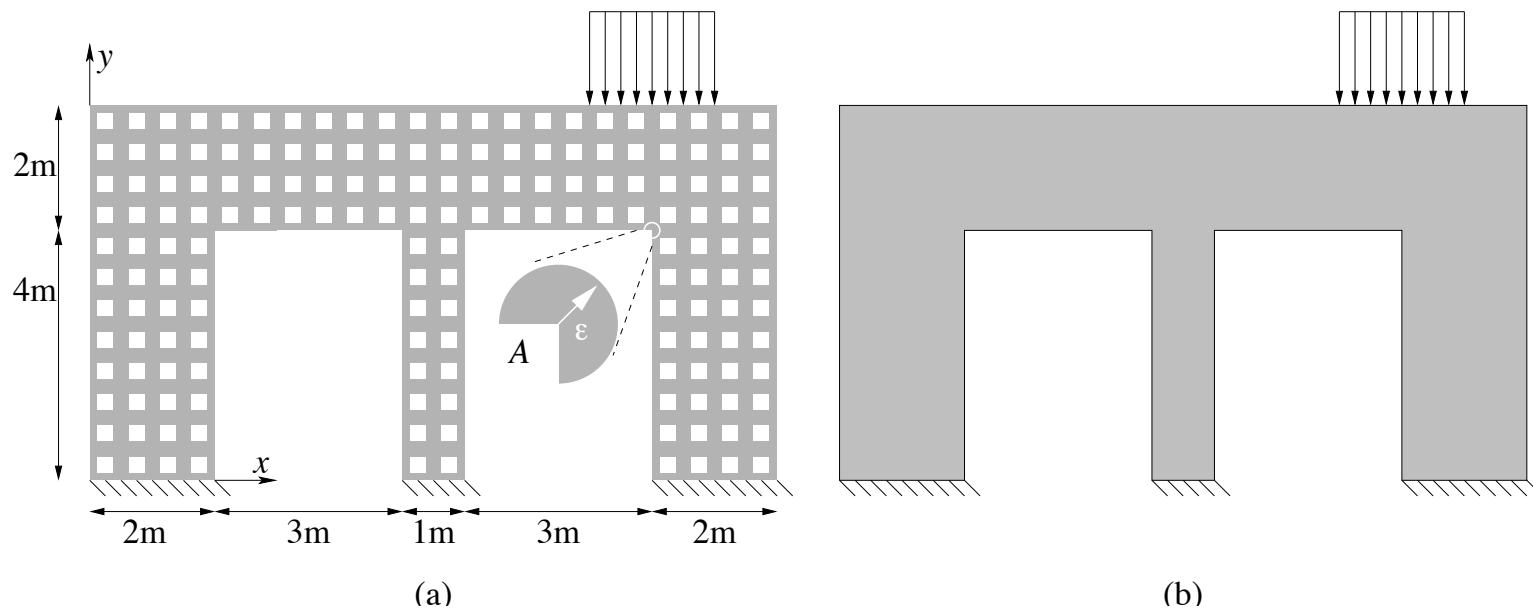
QC (left) and Goals (right) meshes at load step 27.
(Right after the dislocation nucleation)

The numbers of atoms in the QC mesh and the Goals mesh are
1629 and 3452.

3. CONCLUSIONS

- ▶ Estimates of modeling errors in quantities of interest provide a basis for comparing results produced by models of different scales.
- ▶ The theory provides a rigorous approach for controlling the modeling error through adaptive modeling driven by GOALS algorithms.
- ▶ Examples demonstrate a wide range of possible applications.

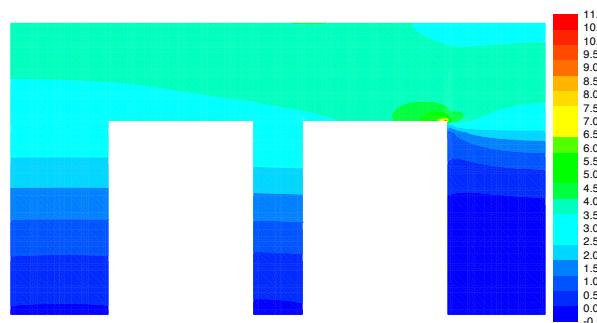
2.1 APPLICATIONS - PERFORATED MATERIAL



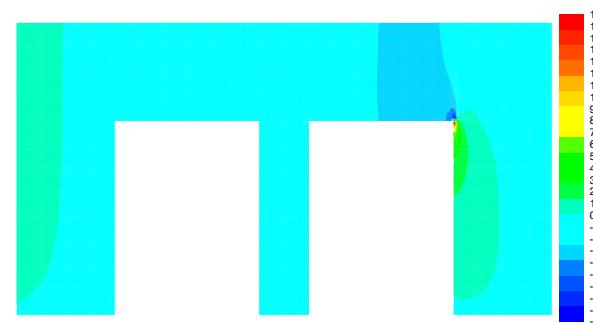
Quantity of Interest:

$$Q(v) = \frac{1}{|A|} \int_A \sigma_{yy}(v) dx$$

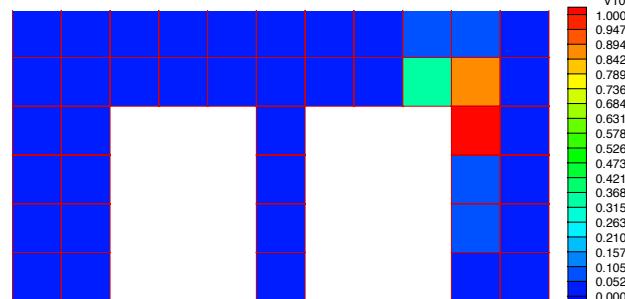
2.1 APPLICATIONS - PERFORATED MATERIAL



$w^0 : x \text{ comp.}$



$w^0 : y \text{ comp.}$



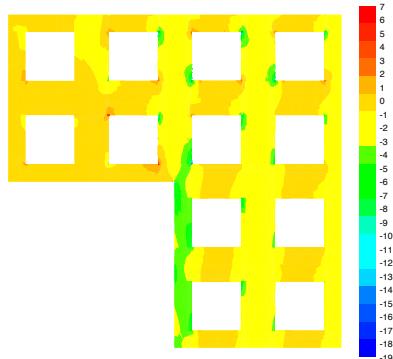
$$Q(\mathbf{v}) = \frac{1}{|A|} \int_A \sigma_{yy}(\mathbf{v}) dx$$

Normalized error indicators β_k

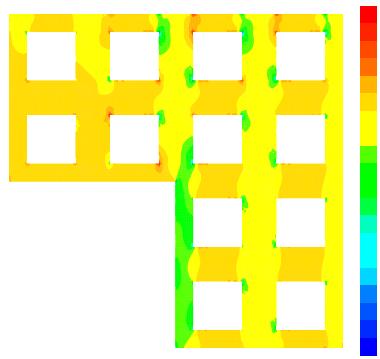
2.1 APPLICATIONS - PERFORATED MATERIAL

The σ_{yy} field:

Local Solution



Fine-scale Solution



$$Q(\tilde{u}) = \mathbf{-0.27 \text{ GPa}}$$

$$Q(u) = \mathbf{-0.25 \text{ GPa}}$$

Fine-scale problem: $\approx 110,000$ dofs

Homogenized solution: $\approx 10,000$ dofs

Local problem: $\approx 13,000$ dofs

2.3. PLATE AND SHELL MODELS: EIGENFREQUENCY ANALYSIS

Find $u(x)$ such that

$$\nabla \cdot \sigma + \omega^2 \rho u = 0 \quad \text{in } \Omega$$

where

$$\sigma = \frac{1}{2}E(\nabla u + \nabla u^T)$$

Boundary conditions:

$$u = 0 \quad \text{on } \Gamma_D$$

$$\sigma \cdot n = 0 \quad \text{on } \Gamma_N$$

E = Elasticity tensor

ρ = density

Frequency = $f = \omega/2\pi$

Generalized eigenvalue problem:

Find (u, λ) such that

$$B(u, v) = \lambda M(u, v) \quad \forall v \in V$$

where

$$V = \{v \in (H^1(\Omega))^d; v = 0 \text{ on } \Gamma_u\}$$

$$B(u, v) = \int_{\Omega} \nabla v : E \nabla u \, dx$$

$$M(u, v) = \int_{\Omega} \rho u \cdot v \, dx$$

$$f = \frac{\omega}{2\pi} = \frac{\sqrt{\lambda}}{2\pi}$$

2.3. ERROR IN EIGENVALUE

Let $U = (u, \lambda)$ denote eigenpairs.

Assume $Q(U) = \lambda$. The dual solutions are given by:

$$\begin{aligned} P &= (u, 0) \\ P_h &= (u_h, 0) \end{aligned} \} \implies \Sigma = P - P_h = (u - u_h, 0) = (e, 0)$$

Error in Eigenvalue:

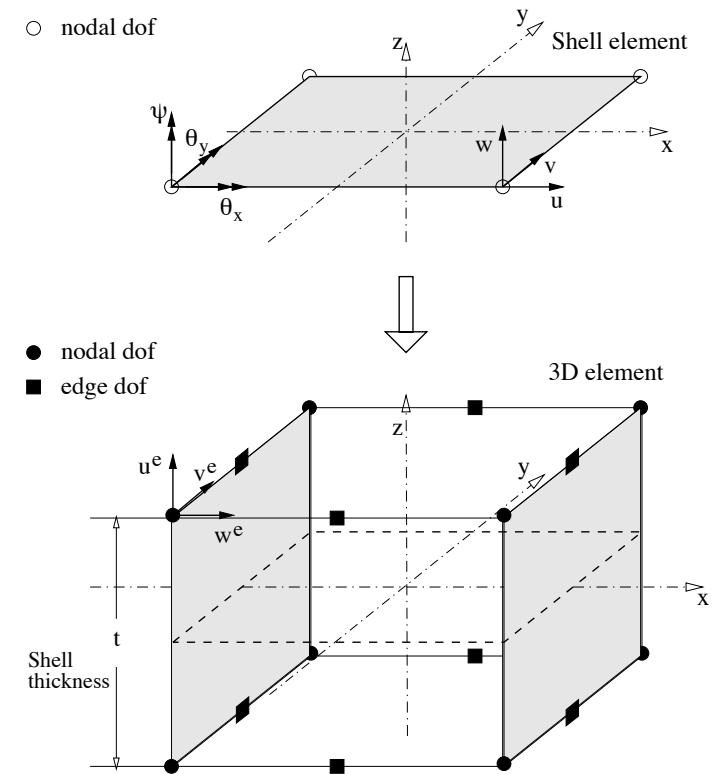
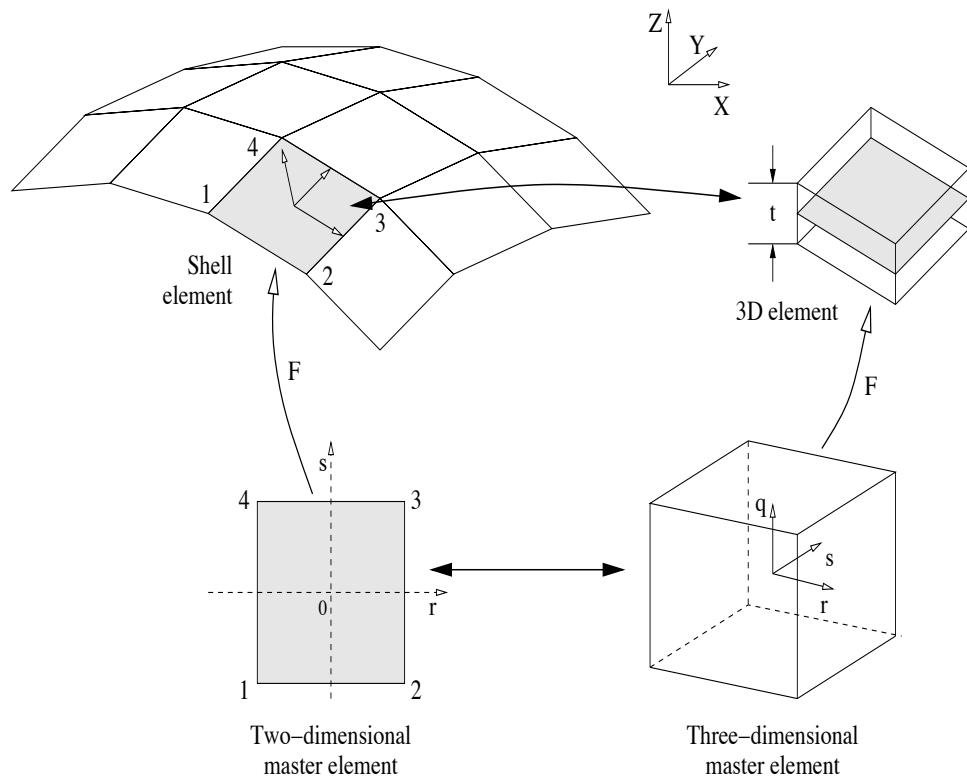
$$\lambda - \lambda_h = \mathcal{R}(U_h; P_h) + \mathcal{R}(U_h; \Sigma) + \Delta$$

with

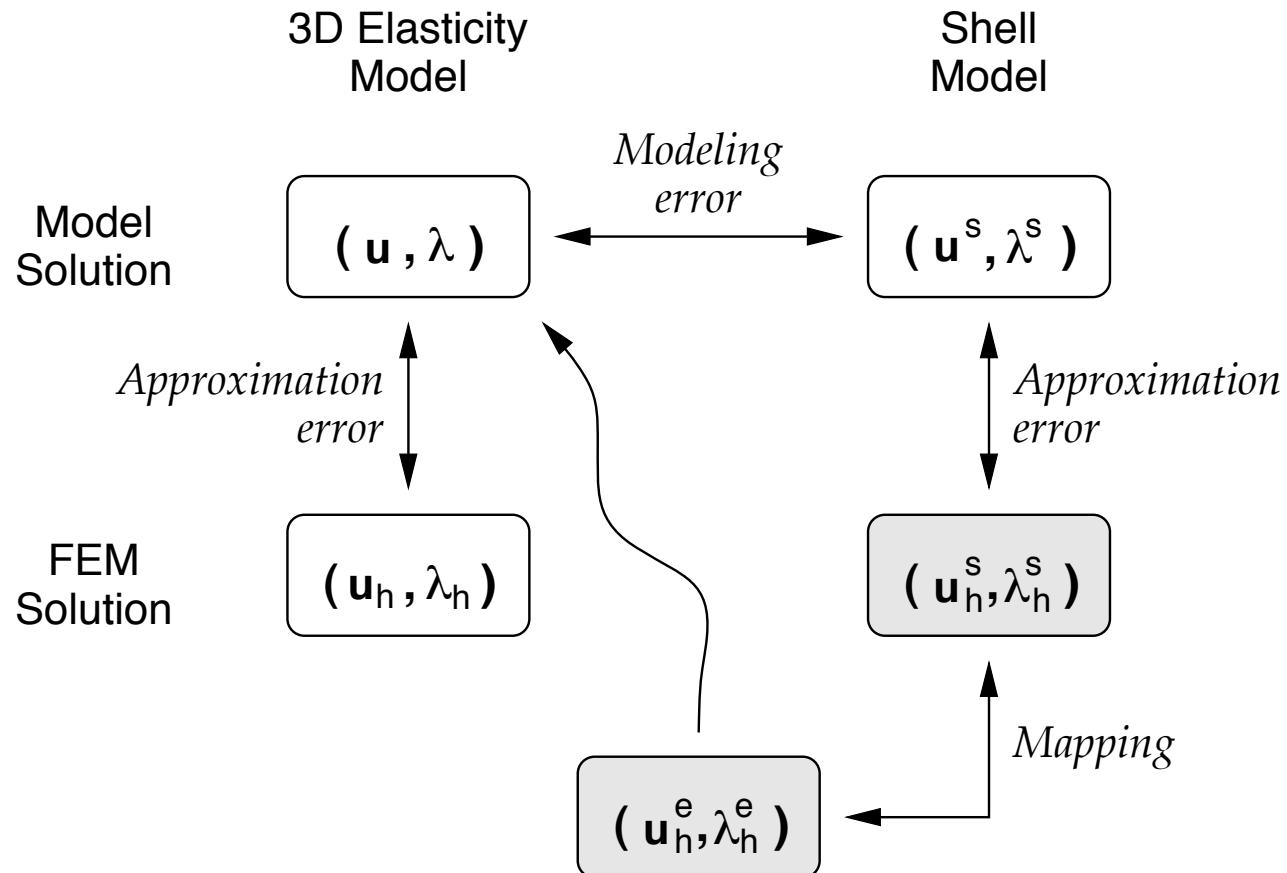
$$\begin{aligned} \mathcal{R}(U_h; P_h) &= B(u_h, u_h) - \lambda_h M(u_h, u_h) \\ \mathcal{R}(U_h; \Sigma) &= B(u_h, e) - \lambda_h M(u_h, e) \end{aligned}$$

*Oden, Prudhomme, Westermann, Bass, and Botkin, M3AS 13 (2003).

2.3. EIGENFREQUENCY FOR SHELL STRUCTURES



2.3. EIGENFREQUENCY FOR SHELL STRUCTURES

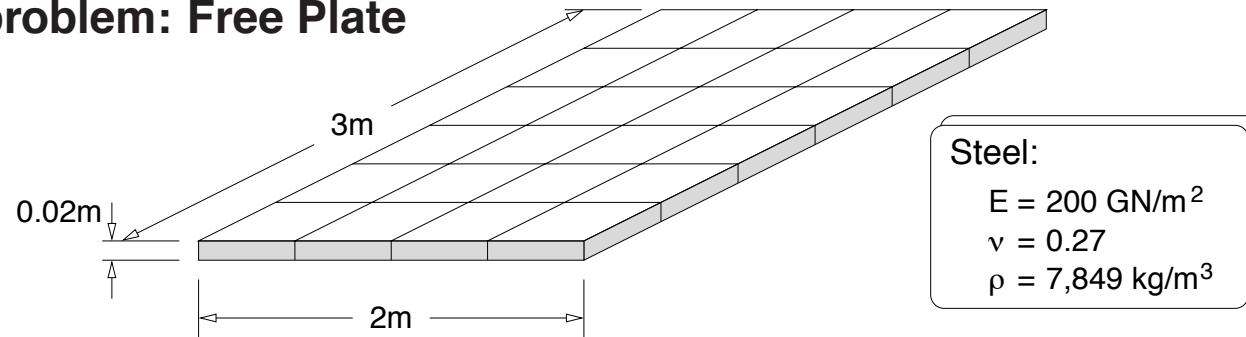


2.3. ALGORITHM

1. Compute (u_h^s, λ_h^s) using the shell model.
2. Transform u_h^s into a 3D displacement field.
3. Extract eigenpair (u_h^e, λ_h^e) on brick elements.
4. Compute error estimates:
 - ☞ Compute $\mathcal{R}(U_h^e; P_h^e)$ since (u_h^e, λ_h^e) does not necessarily satisfy the orthogonality property.
 - ☞ Estimate $\mathcal{R}(U_h; \Sigma)$ as in 3D elasticity.
5. Compute error estimates in natural frequencies.

2.3. EIGENFREQUENCY FOR SHELL STRUCTURES

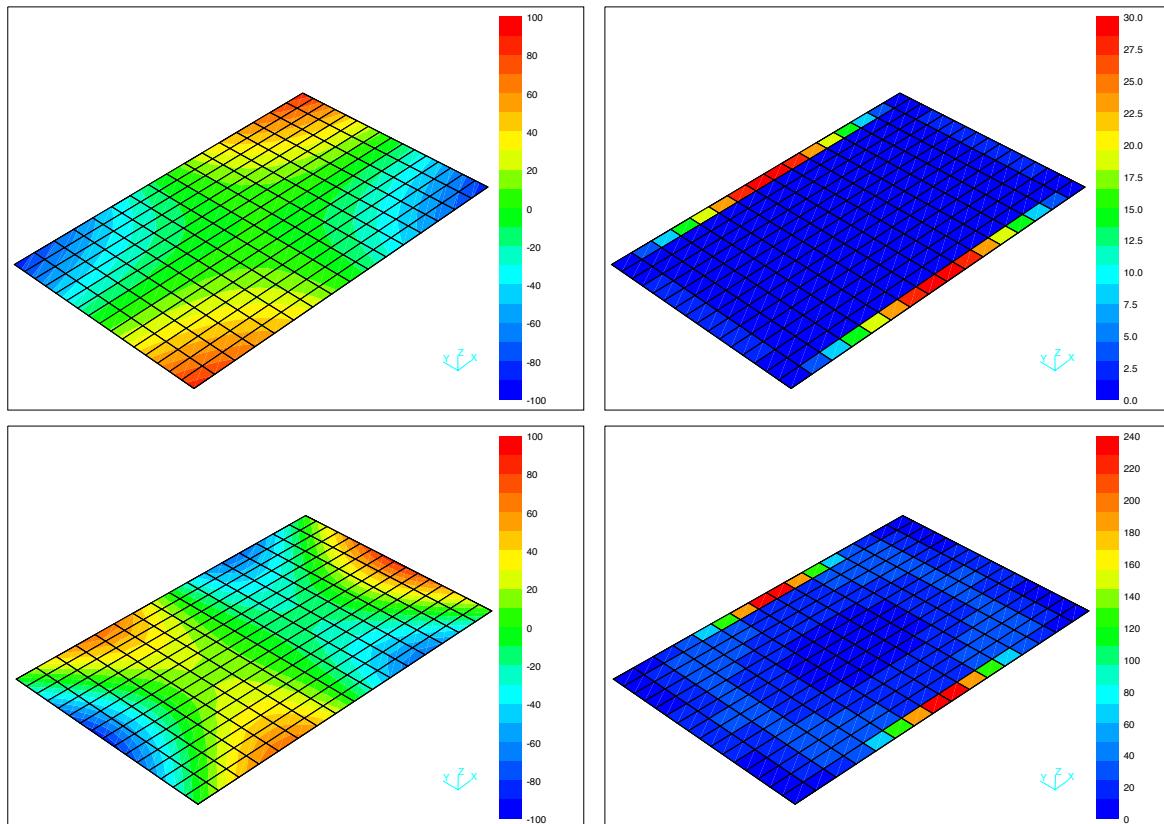
Model problem: Free Plate



Frequency number	Mesh (6,4)		Mesh (12,8)		Mesh (16,16)		Mesh (24,16)	
	f_h^s	$f_h^s + \eta^f$	f_h^s	$f_h^s + \eta^f$	f_h^s	$f_h^s + \eta^f$	f_h^s	$f_h^s + \eta^f$
$f_1 = 10.95$	10.10	14.07	10.71	11.24	10.85	11.06	10.88	10.96
$f_2 = 11.56$	10.68	13.42	11.32	11.71	11.42	11.62	11.49	11.57
$f_3 = 25.14$	21.99	39.34	24.28	26.42	24.74	25.51	24.90	25.24
$f_4 = 26.75$	22.98	35.76	25.64	27.49	26.45	26.83	26.44	26.82
$f_5 = 31.26$	26.54	47.80	29.94	32.75	30.64	31.79	30.90	31.39

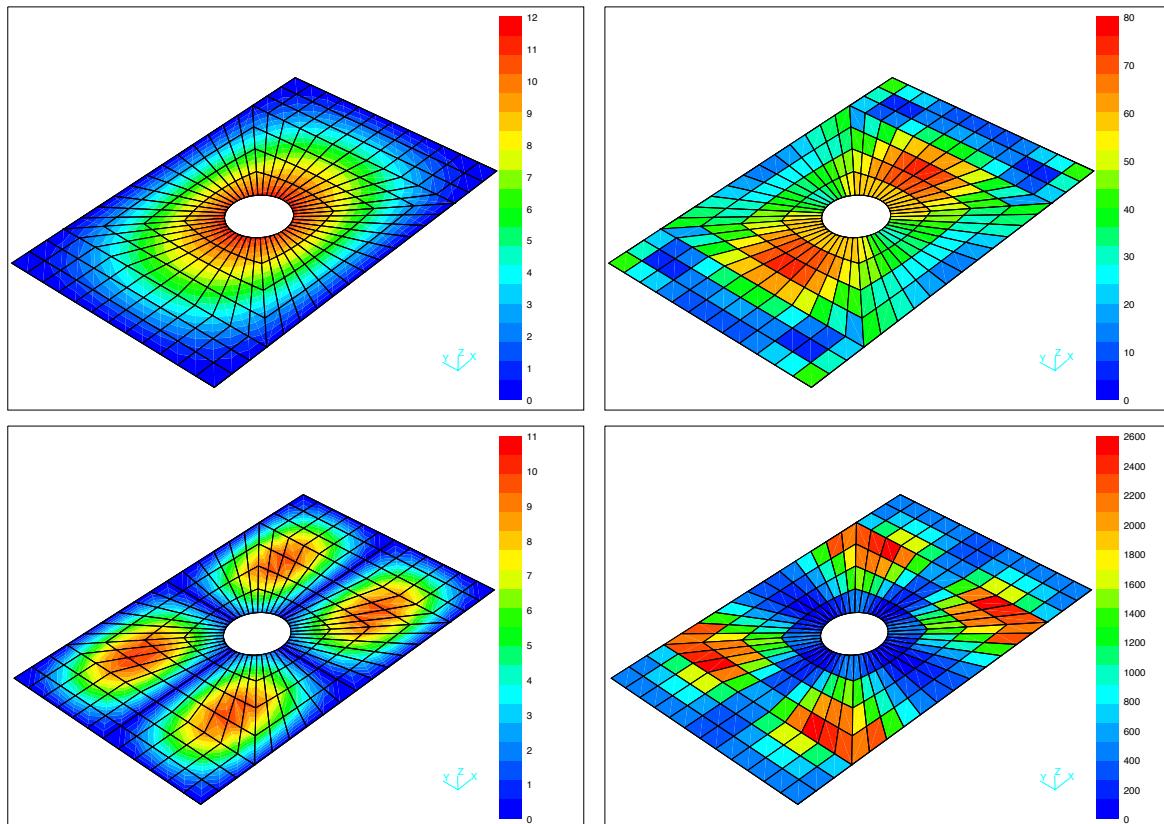
Computed and estimated frequencies f_h^s and $f_h^s + \eta^f$ using shell analysis.

2.3. EIGENFREQUENCY FOR SHELL STRUCTURES



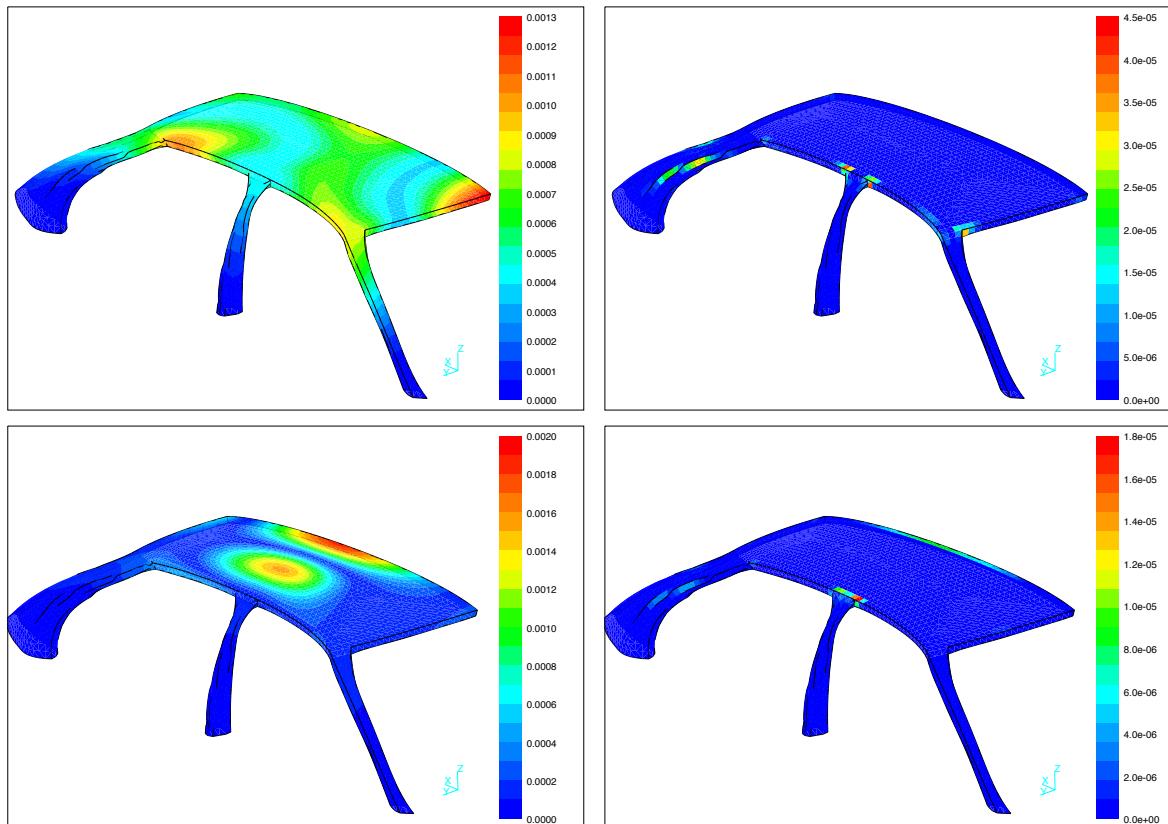
Eigenmode (left) and error distribution (right) for f_1 (top) and f_5 (bottom).

2.3. EIGENFREQUENCY FOR SHELL STRUCTURES



Eigenmode (left) and error distribution (right) for f_1 (top) and f_5 (bottom).

2.3. EIGENFREQUENCY FOR SHELL STRUCTURES



Eigenmode (left) and error distribution (right) for f_4 (top) and f_5 (bottom).